Thermodynamic entropy and excess information loss in dynamical systems with time-dependent Hamiltonian

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Abstract

We study a dynamical system with time dependent Hamiltonian by numerical experiments so as to find a relation between thermodynamics and chaotic nature of the system. Excess information loss, defined newly based on Lyapunov analysis, is related to the increment of thermodynamic entropy. Our numerical results suggest that the positivity of entropy increment is expressed by the principle of the minimum excess information loss.

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Boltzmann found a famous formula which relates thermodynamic entropy with a number of states in microscopic systems. While the formula was practically well-established, there have been discussions on its justification over the century [1]. In particular, understanding the origin of irreversibility seems to be controversial even to the present knowledge. On the other hand, owing to development of computational circumstance, we can easily investigate numerical solutions to equations of motion in Hamiltonian systems with a high degrees of freedom. Thus, through numerical experiments, it may be possible to get new insights for the relation between thermodynamics and dynamical systems. In particular, we are concerned with a question how thermodynamic entropy is related to notions of dynamical system theory.

We study numerically a Fermi-Pasta-Uram (FPU) model [2], whose Hamiltonian is given by

$$H(\{q_i\},\{p_i\};g)=\sum_{i=1}^{N}[\frac{1}{2}p_i^2+\frac{1}{2}(q_{i+1}-q_i)^2+\frac{g}{4}(q_{i+1}-q_i)^4], \tag{1}$$

where g is a time dependent parameter. Then, the evolution equations for $(\{q_i\},\{p_i\})$ are written as

$$\frac{dq_i}{dt}=p_i, \tag{2}$$

$$\frac{dp_i}{dt}=(q_{i+1}-q_i)+g(q_{i+1}-q_i)^3-(q_i-q_{i-1})-g(q_i-q_{i-1})^3. \tag{3}$$

We assume periodic boundary conditions, that is, q_0 and q_{N+1} in Eq.(3) satisfy $q_0=q_N$ and $q_{N+1}=q_1$. We also assume that the values of conserved quantities $\sum_i q_i$ and $\sum_i p_i$ are zero. We solve numerically Eqs.(2) and (3) by the 4-th order symplectic integrator method with a time step $\delta t=0.005$ [4]. When we are concerned with the system in the thermodynamic limit, numerical calculation should be done with several values of N. In the argument below, results for $N=5$ and $N=20$ will be presented.

We first discuss the case that g takes a constant value, say g_0. We assume that initial conditions are chosen from the micro-canonical ensemble with an energy E_0. When E_0g_0 is sufficiently large, the system exhibits high-dimensional chaos. As an example of such

parameter values, $(E_0, g_0) = (1.0, 10.0)$ is assumed. The nature of high-dimensional chaos is characterized by Lyapunov spectrum and Kolmogorov-Sinai (KS) entropy. We first review briefly how to obtain them numerically. This is a well-known fact, but will help us to introduce a new quantity "excess information loss" later.

Let a solution to Eqs.(2) and (3) denote $\Gamma(t) = (q_1(t), p_1(t), q_2(t), p_2(t), \cdots, q_N(t), p_N(t))$. In Lyapunov analysis, divergence and convergence of distance between neighboring orbits are described by time evolution of a set of $2N$ orthogonal unit vectors, $\{\mathbf{e}_i\}_{i=1}^{2N}$, each of which obeys the linearized equations of Eqs.(2) and (3). By employing the Gram-Schmidt procedure, which was developed as a numerical calculation method for Lyapunov exponents [5], the evolution of $\mathbf{e}_i$, $\hat{T}(t,0)\mathbf{e}_i$, is expressed by

$$\hat{T}(t,0)\mathbf{e}_i = \sum_j \hat{F}(t,0)\mathbf{e}_j R_{ji}(t,0), \tag{4}$$

where R_{ij} is the (i,j) element of an upper triangle matrix $\hat{R}$, and $\hat{F}(t,0)$ is an orthogonal matrix. We can find the matrices $\hat{R}$ and $\hat{F}$ so that the diagonal elements of $\hat{R}$ are positive. Note that $\{\hat{F}(t,0)\mathbf{e}_i\}_{i=1}^{2N}$ gives an orthogonal set defined in the tangent space at the point $\Gamma(t)$. From the definition of the matrix $\hat{R}$, the j-dimensional parallelepiped volume spanned by $\{\hat{T}(t,0)\mathbf{e}_i\}_{i=1}^{j}$ is calculated as

$$\Omega_j(t,0;\{\mathbf{e}_i\}) = \Pi_{i<j} R_{ii}(t,0). \tag{5}$$

The i-th Lyapunov exponent λ_i is then defined by

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \log \frac{\Omega_i(t,0;\{\mathbf{e}_i\})}{\Omega_{i-1}(t,0;\{\mathbf{e}_i\})}. \tag{6}$$

All Lyapunov exponents for the model in question are shown in Fig. 1. Note that there are four zeros due to the periodic boundary conditions. Further, the KS entropy h is given by [3]

$$h = \sum_{\lambda_i>0} \lambda_i. \tag{7}$$

Since the number of positive Lyapunov exponents is $N-2$, the KS entropy is expressed by

$$h = \lim_{t\to\infty} \frac{1}{t} \log \Omega_{N-2}(t, 0; \{\mathbf{e}_i\}). \tag{8}$$

We also define a special orthonormal set $\{\mathbf{e}_i^*\}_{i=1}^{2N}$ at a point $\Gamma(0)$ by

$$\mathbf{e}_i^* = \lim_{t_b\to-\infty} \hat{F}(0, t_b)\mathbf{e}_i, \tag{9}$$

where $\{\mathbf{e}_i\}$ is an orthonormal set defined in the tangent space at $\Gamma(t_b)$. $\mathbf{e}_i^*$ corresponds to the i-th Lyapunov vector at a point $\Gamma(0)$.

Now, we consider the case that the value of g is changed in time from g_0 to g_1. Especially, we pay attention to two limiting cases of the parameter change, quasi-static process and instantaneous switching process. In a quasi-static limit, the parameter is changed in a slower way than all physical time scales. Since thermodynamic entropy in isolated systems should be kept at constant in quasi-static processes, equi-entropy lines in the (E, g) plane can be obtained numerically by quasi-static processes. Figure 2 shows the equi-entropy line through (E_0, g_0), which is denoted by $E = E_{qs}(g)$. We also define $E_*(E, g)$ by a requirement that $(E_*, 0)$ is on the equi-entropy line through (E, g). Since the FPU model with $g = 0$ is nothing but the harmonic oscillator model, we can evaluate the entropy at (E, g) as

$$S(E, g) = S(E_*(E, g), 0) = (N - 2) \log E_*(E, g), \tag{10}$$

where an additive constant with respect to E_* is omitted, and the Boltzmann constant is assumed to be unity.

Instantaneous switching is the other extreme limit of the parameter change. The value of g is changed instantaneously from g_0 to $g_1 = g_0 + \Delta g$ at $t = 0$. Then, the energy after the switching becomes E_1, whose value depends on the choice of initial conditions. The entropy difference ΔS can be defined by

$$\Delta S = S(E_1, g_1) - S(E_0, g_0), \tag{11}$$

where S is calculated by the formula Eq.(10). In Fig. 3, the average of the entropy difference over initial conditions $\langle \Delta S \rangle$ was plotted against Δg. In the thermodynamic limit, the relative

fluctuation of E_1 becomes negligible and then E_1 can be identified with the averaged value $\langle E_1 \rangle$. Note that $\langle E_1 \rangle$ satisfies

$$\langle E_1 \rangle - E_0 = \left(\frac{dE_{qs}(g)}{dg} \right) (g_1 - g_0). \tag{12}$$

That is, $\langle E_1 \rangle$ is determined in such a way that $(\langle E_1 \rangle, g_1)$ is in the straight line contacting to the equi-entropy line $E = E_{qs}(g)$ at (E_0, g_0). (See Fig. 2.) We also confirmed this statement numerically. Since the equi-entropy line is convex in the (E, g) plane, the entropy difference between the states $(\langle E_1 \rangle, g_1)$ and (E_0, g_0) turns out to be always positive. In fact, in Fig. 3, $S(\langle E_1 \rangle, g_1) - S(E_0, g_0)$ was shown against Δg. One may find that how ΔS approaches to $S(\langle E_1 \rangle, g_1) - S(E_0, g_0)$ as N is increased.

We now attempt to express ΔS at instantaneous switching in terms of notions of dynamical system theory. One may naively expect that thermodynamic entropy is related to KS entropy. In fact, the extensivity of KS entropy suggests a relation with thermodynamics. However, since KS entropy has the same dimension as the inverse of time, the relation is not straightforward. Further, we should notice that KS entropy measures the rate of information loss at a steady state in dynamical systems, while thermodynamic entropy changes only by external action. We thus expect that ΔS is related to the change of information loss brought by the parameter switching. Motivated by this picture, we next define the excess information loss.

Since the parameter is switched instantaneously at $t = 0$, the orbit is not smooth at this time. We thus define a smooth orbits $\Gamma_{st}(t; g_1)$ in such a way that $\Gamma_{st}(t; g_1) = \Gamma(t)$ for $t \geq 0$. The values of Γ_{st} in the other region are determined by the requirement of the smoothness of Γ_{st} at $t = 0$. Note that the orbit $\Gamma_{st}(\ ; g_1)$ is on a new energy surface. Since the two orbits $\Gamma()$ and $\Gamma_{st}(\ ; g_1)$ intersect at $\Gamma(0)$, two sets of Lyapunov vectors, denoted by $\mathbf{e}_i^*(g_0)$ and $\mathbf{e}_i^*(g_1)$ respectively, are defined there by the time evolution along the two orbits $\Gamma()$ and $\Gamma_{st}(\ ; g_1)$ from a sufficiently long ago. (See Eq.(9).) Then, recalling the definition of KS entropy given by Eq.(8), we can interpret $\log \Omega_{N-2}(t, 0; \{\mathbf{e}_i^*(g_0)\})$ as the actual information loss during a time interval $[0, t]$, because the set of Lyapunov vectors $\{\mathbf{e}_i^*(g_0)\}$ at $t = 0$ is

associated with the actual orbit $\Gamma()$. On the contrary, the quantity $\log \Omega_{N-2}(t, 0; \{\mathbf{e}_i^*(g_1)\})$ corresponds to the information loss for the virtual orbit $\Gamma_{st}(\ ; g_1)$ on the new energy surface. We now define the 'excess information loss' brought by the parameter change as

$$H_{ex} = \lim_{t \to \infty} [\log \Omega_{N-2}(t, 0; \{\mathbf{e}_i^*(g_0)\}) - \log \Omega_{N-2}(t, 0; \{\mathbf{e}_i^*(g_1)\})]. \tag{13}$$

In Fig. 4, the average of H_{ex} over initial conditions, $\langle H_{ex} \rangle$, was plotted against Δg. Comparing this graph with that in Fig. 3, one may doubt that $\langle H_{ex} \rangle$ has no direct relation with $\langle \Delta S \rangle$. In particular, behaviors for $\Delta g \to 0$ are qualitatively different: $\langle H_{ex} \rangle \sim O(\Delta g)$, while $\langle \Delta S \rangle \sim O((\Delta g)^2)$. This property implies that the excess information loss in the quasi-static process $g_0 \to g_1$, denoted by $\langle H_{ex} \rangle_{qs}$, takes a nonzero value. $\langle H_{ex} \rangle_{qs}$ may be calculated as

$$\langle H_{ex} \rangle_{qs} = \int_{g_0}^{g_1} dg \Psi(E_{qs}(g), g), \tag{14}$$

where Ψ is determined by an infinitely small jump process $g \longrightarrow g + \delta g$ at the energy $E_{qs}(g)$. Now, it seems natural to assume the decomposition of $\langle H_{ex} \rangle$ in the form

$$\langle H_{ex} \rangle = \langle H_{ex} \rangle_{qs} + c \langle \Delta S \rangle, \tag{15}$$

where c_0 is a constant. In order to check the validity of Eq.(15), we performed the reversed experiments in which the parameter g is changed from g_1 to g_0 with the initial energy $E_{qs}(g_1)$. We then obtained $\langle H_{ex} \rangle'$ and $\langle \Delta S \rangle'$. We assume the relation Eq. (15) for the reversed experiment, that is,

$$\langle H_{ex} \rangle' = \langle H_{ex} \rangle'_{qs} + c \langle \Delta S \rangle', \tag{16}$$

where

$$\begin{aligned} \langle H_{ex} \rangle'_{qs} &= \int_{g_1}^{g_0} dg \Psi(E_{qs}(g), g), & (17) \\ &= -\langle H_{ex} \rangle_{qs}. & (18) \end{aligned}$$

Therefore, from Eqs.(15), (16) and (18), we obtain

$$\langle H_{ex}\rangle + \langle H_{ex}\rangle' = c(\langle \Delta S\rangle + \langle \Delta S\rangle'). \tag{19}$$

This relation was checked numerically. As shown in Fig. 5, Eq. (19) seems valid with $c = 0.5$. We thus expect

$$\langle H_{ex}\rangle = \langle H_{ex}\rangle_{qs} + \frac{1}{2}\langle \Delta S\rangle. \tag{20}$$

This is the main claim of the present paper. It is worthwhile noting that the positivity of the entropy difference is expressed by the principle of the minimum excess information loss.

In closing the paper, we introduce related studies. Recently, a relation between phenomenology of nonequilibrium steady states and dynamical system theory has been discussed by employing deterministic models with a thermostat or with open boundaries [6–9]. In particular, an entropy production ratio is expressed in terms of KS entropy. This may have correspondence with Eq.(20). (Note that we never discuss nonequilibrium steady states, but transitions between equilibrium states.) Further, Oono and Palconi have developed new phenomenology of steady state thermodynamics [10], in which 'excess heat' plays an important role in the definition of the entropy at a nonequilibrium steady state. When we replace a term 'heat' in their theory by 'information', we find much similarity between two theories. In order to discuss relations among the apparently different theories, we need to present a mathematical proof of Eq.(20) together with the positivity of ΔS.

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FIGURES

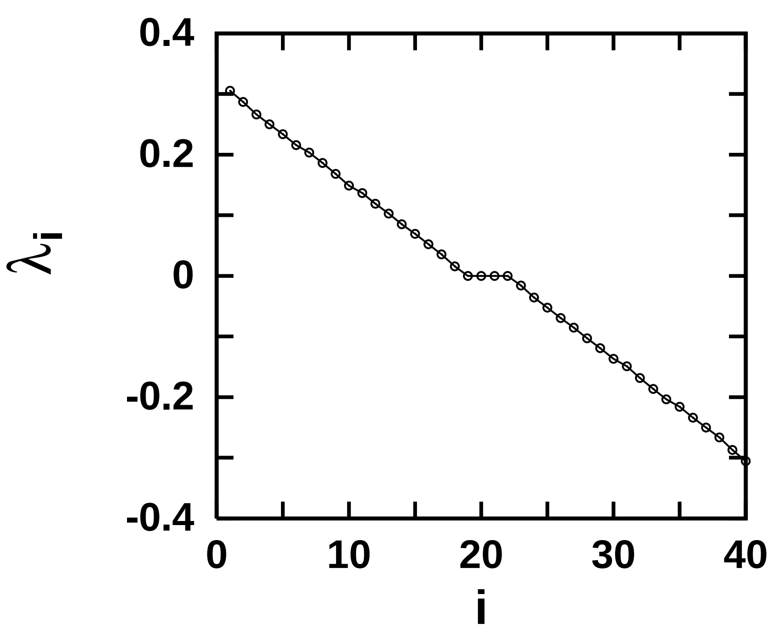
FIG. 1. Lyapunov spectrum. $N = 20$. $\Omega_j(t,0)$ at $t = 10^5$ was measured to evaluate the Lyapunov exponents.

FIG. 2. Averaged energy after instantaneous switching processes and the equi-entropy line through $(E, g) = (1.0, 10.0)$.

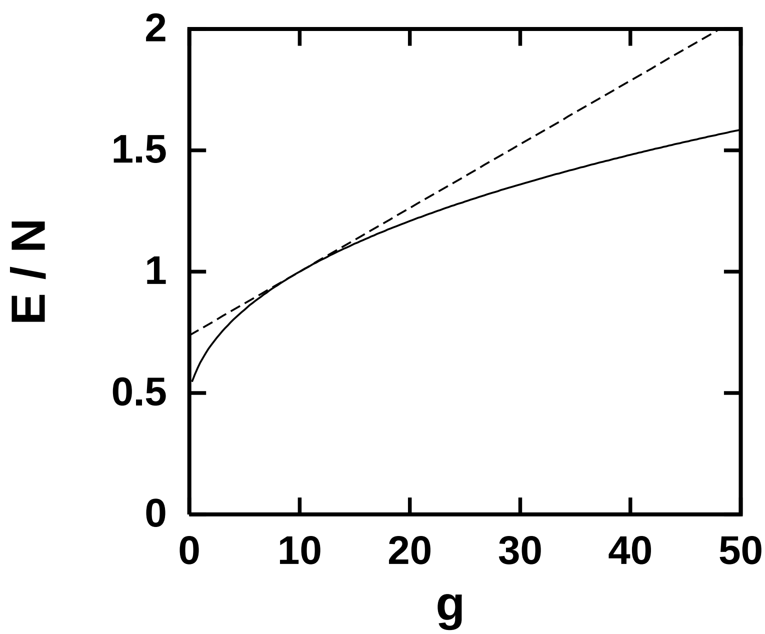
FIG. 3. Entropy difference versus Δg. N=20. Solid line shows $S(\langle E_1\rangle, g_1) - S(E_0, g_0)$. Square and filled circle symbols represent $\langle S(E_1, g_1)\rangle - S(E_0, g_0)$ for $N = 5$ and $N = 20$, respectively.

FIG. 4. H_{ex} versus Δg. Square and filled circle symbols represent the data for $N = 5$ and $N = 20$, respectively. H_{ex} was evaluated with checking the convergence.

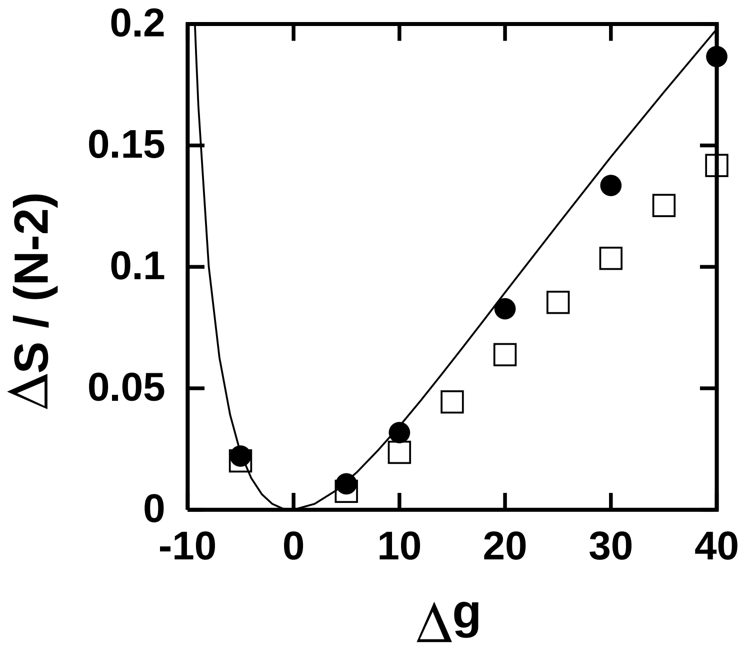
FIG. 5. $\langle H_{ex}\rangle + \langle H_{ex}\rangle'$ versus $\langle \Delta S\rangle + \langle \Delta S\rangle'$. Square and filled circle symbols represent the data for $N = 5$ and $N = 20$, respectively. The dashed line shows $\langle H_{ex}\rangle + \langle H_{ex}\rangle' = 1/2[\langle \Delta S\rangle + \langle \Delta S\rangle']$.



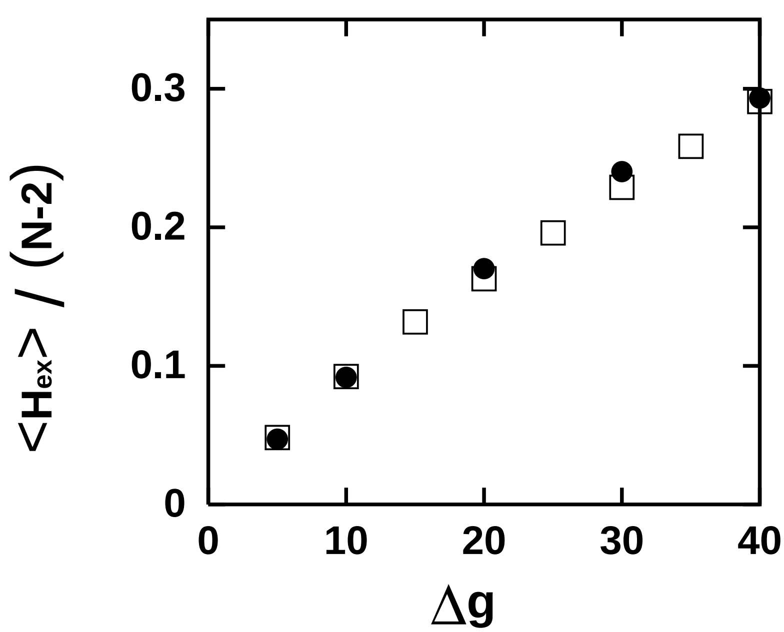
S.Sasa and T.S.Komatsu Figure 1.



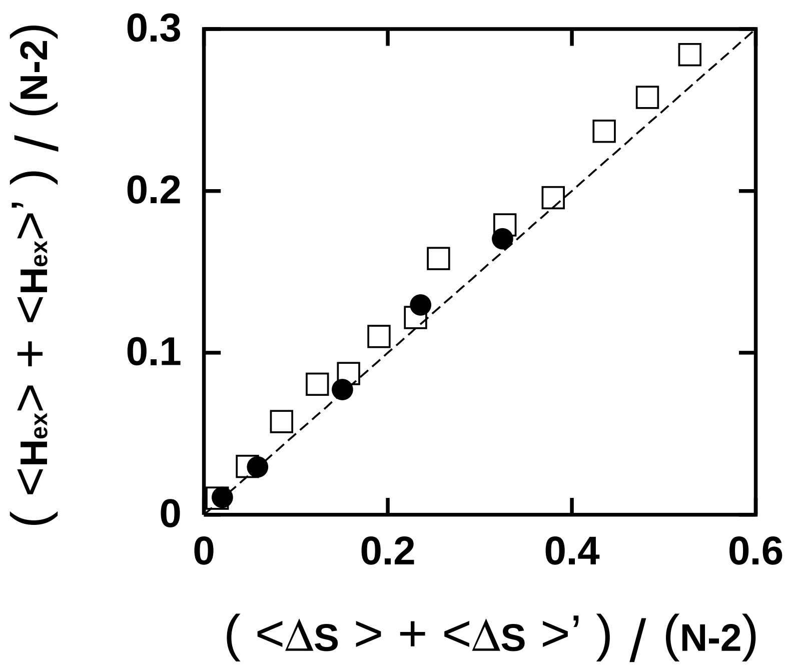
S.Sasa and T.S.Komatsu Figure 2.



S.Sasa and T.S.Komatsu Figure 3.



S.Sasa and T.S.Komatsu Figure 4.



S.Sasa and T.S.Komatsu Figure 5.